# Stochastic model for protein B-factor prediction

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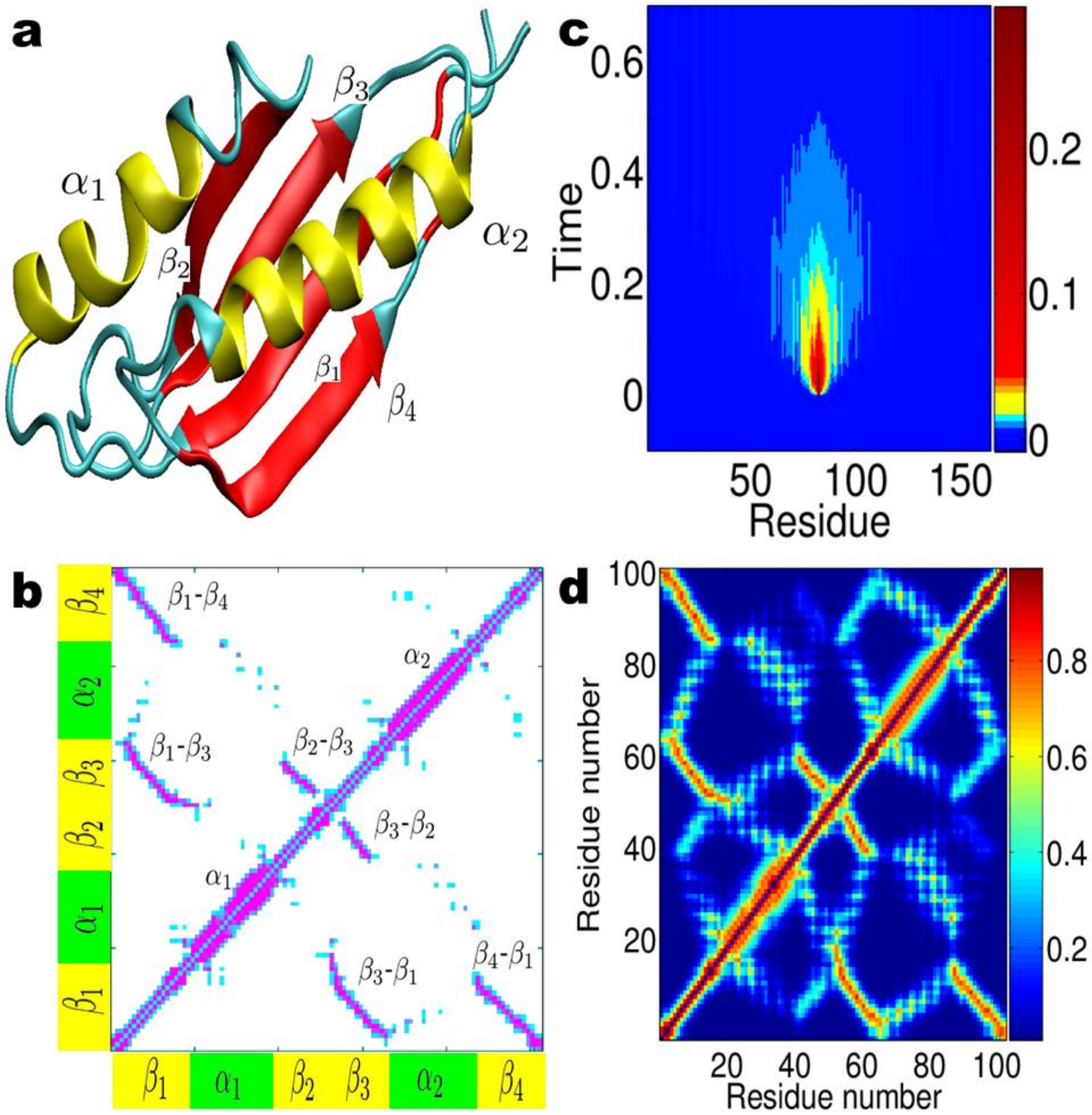
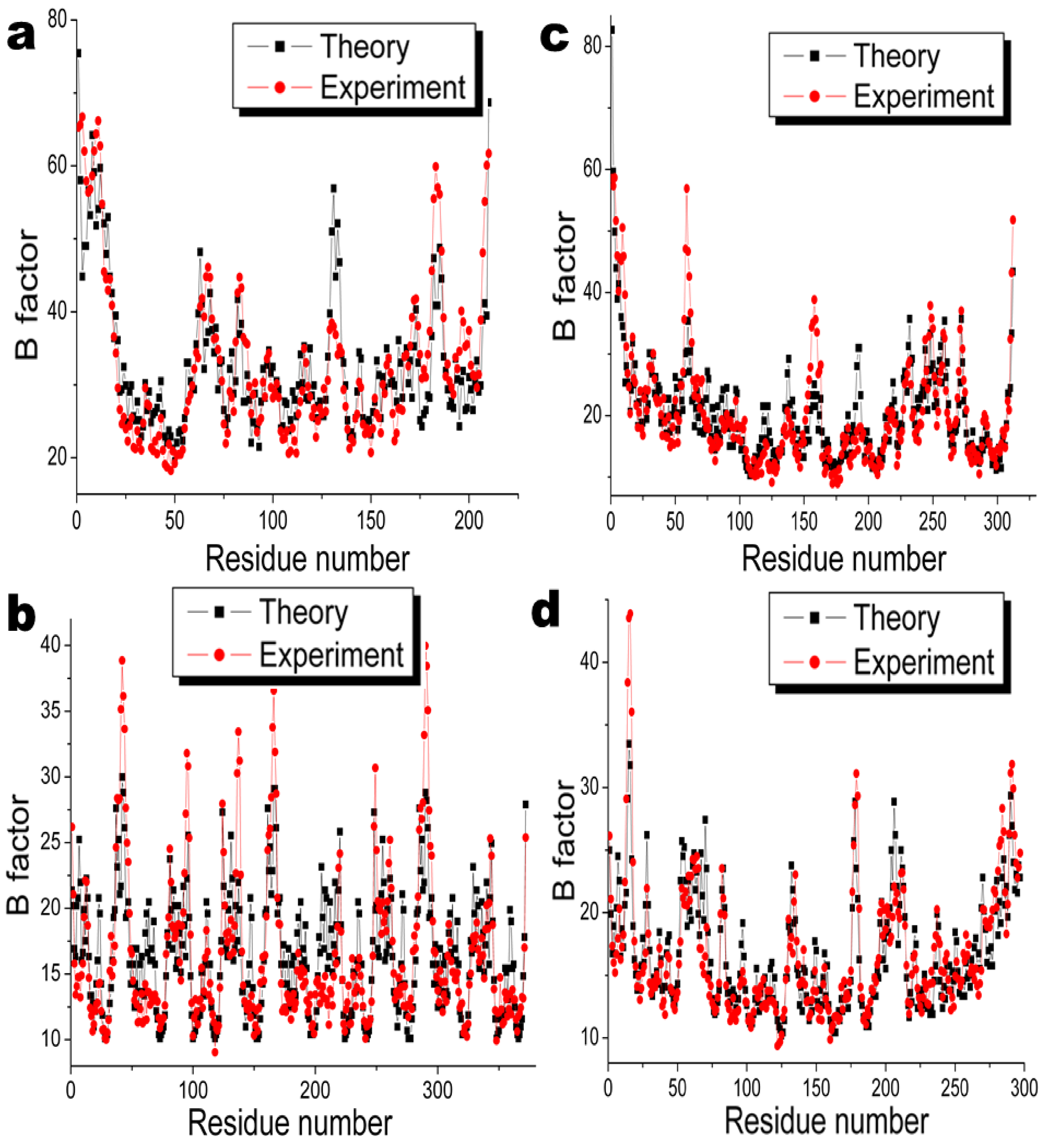
## Introduction

**Protein flexibility is an intrinsic property and plays a fundamental role in protein functions. Computational analysis of protein flexibility is crucial to protein function prediction, macromolecular flexible docking, and rational drug design. Most current approaches for protein flexibility analysis are based on Hamiltonian mechanics and matrix diagonalization. We introduce a stochastic model for protein flexibility analysis. The essential idea is to analyze the free induction decay of a perturbed protein structural probability, which satisfies the master equation. The transition probability matrix is constructed by using probability density estimators including monotonically decreasing radial basis functions. The proposed model by-passes matrix diagonalization. We show that the proposed stochastic model gives rise to some of the best predictions of Debye-Waller factors or B factors for three sets of protein data introduced in the literature.**





## References

*Kelin Xia and G.W. Wei,* Stochastic model for protein flexibility analysis, *Physical Review E, 88, 062709, 2013.*

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